

The rooting issue for a lattice fermion formulation similar to staggered fermions but without taste mixing

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Abstract

To investigate the viability of the 4th root trick for the staggered fermion determinant in a simpler setting, we consider a two taste (flavor) lattice fermion formulation with no taste mixing but with exact taste-nonsinglet chiral symmetries analogous to the taste-nonsinglet $U(1)_A$ symmetry of staggered fermions. M. Creutz's objections to the rooting trick apply just as much in this setting. To counter them we show that the formulation has robust would-be zero-modes in topologically nontrivial gauge backgrounds, and that these manifest themselves in a viable way in the rooted fermion determinant and also in the disconnected piece of the pseudoscalar meson propagator as required to solve the $U(1)$ problem. Also, our rooted theory is heuristically seen to be in the right universality class for QCD if the same is true for an unrooted mixed fermion action theory.

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I. INTRODUCTION

The use of dynamical staggered fermions in lattice QCD simulations has made it possible to obtain results with unprecedented high precision [1, 2, 3]. However, this approach is controversial due to the use of the “4th root trick”: A staggered lattice fermion corresponds to 4 continuum fermion flavors (nowadays called tastes to distinguish them from the actual quark flavors), so the fermion determinant for each dynamical quark flavor is represented by the 4th root of the corresponding staggered fermion determinant. Since this formulation is not manifestly a local lattice field theory there is a danger that it might not be in the right universality class for QCD. (In fact it has been argued [4] that this lattice theory is necessarily non-local but with locality being restored in the continuum limit [5].¹) Because of the high stakes, this has become a prominent, hotly debated issue in the lattice community. E.g., it has been the topic of 5 plenary talks at the last 4 annual lattice field theory conferences; the corresponding proceedings papers [8, 9, 10, 11, 12] can be consulted for reviews from various perspectives.

While the results to date are in excellent, unprecedented agreement with experiment, a major question regarding the 4th root trick for staggered fermions is whether it can work in situations where chirality is important. This includes in particular producing the large mass of the η' meson where existence of fermionic zero-modes with definite chirality and their connection with topological charge of lattice gauge fields via the Index Theorem plays an essential role [13].² M. Creutz has argued against this in a series of papers [17, 18, 19, 20, 21] based on the fact that the taste-nonsinglet $U(1)$ chiral symmetry of staggered fermions implies properties of the rooted staggered fermion determinant that do not hold for a genuine single-flavor fermion determinant. The subsequent rebuttals of these arguments [22, 23] rely to a large extent on invoking full taste symmetry restoration on the continuum limit. However, Creutz challenges whether this can actually occur in a way that correctly reproduces nonperturbative effects connected with chirality. In this situation it is desirable

¹ In the free field case (at least for $m \neq 0$) the rooted staggered formulation corresponds to a local field theory already at non-vanishing lattice spacing [6], as was also confirmed numerically [7].

² Efforts to calculate the η' mass to high precision with dynamical staggered fermions are currently underway [14, 15]. In the meantime, encouraging evidence that this formulation is able to correctly reproduce topological aspects of QCD has been given in Ref. [16] where results for the topological susceptibility were presented.

to have a simpler setting where the same issues arise and where they can be studied more explicitly. We provide and study such a setting in the present paper.

The paper is organized as follows. In sect. II we contrast a general mixed fermion formulation with a rooted formulation based on a 2-taste lattice Dirac operator without taste-mixing, showing heuristically that if the former is in the right universality class for QCD then so is the latter. In sect. III we introduce the specific 2-taste lattice Dirac operator with exact taste-nonsinglet chiral symmetries on which the rooted formulation studied in this paper is based. In sect. IV we study the properties of the single-flavor fermion formulations based on the 1-taste lattice Dirac operators making up our 2-taste operator, and use this to derive properties of the rooted formulation based on the latter. In sect. V we discuss the pseudo-scalar propagator in the rooted formulation, and conclude with a discussion in sect. VI. A relation between, and differences between, our 2-taste formulation and the 2-flavor Wilson fermion theory with twisted mass is discussed in an appendix.

II. PRELUDE: MIXED FERMION ACTION VERSUS A ROOTED FORMULATION

We begin with some general remarks on generating functionals for lattice fermions (in a fixed gauge field background, in Euclidean spacetime). For a single quark flavor described by a lattice Dirac operator D_1 the generating functional is

$$\begin{aligned} Z_f(\eta, \bar{\eta}) &= \int d\psi d\bar{\psi} e^{-\bar{\psi} D_1 \psi + \bar{\psi} \bar{\eta} + \eta \psi} \\ &= \det D_1 e^{\bar{\eta} D_1^{-1} \eta} \end{aligned} \tag{1}$$

For a “mixed fermion action” where the sea quark is described by D_1 and the valence quark by another lattice Dirac operator D_2 the generating functional becomes

$$Z_{f,mixed}(\eta, \bar{\eta}) = \det D_1 e^{\bar{\eta} D_2^{-1} \eta} \tag{2}$$

Writing this as

$$Z_{f,mixed}(\eta, \bar{\eta}) = e^{\Delta S} \det D_2 e^{\bar{\eta} D_2^{-1} \eta} \tag{3}$$

where

$$\Delta S = Tr \log D_1 - Tr \log D_2 \tag{4}$$

we see that the full lattice QCD theory with mixed fermion action is equivalent to the lattice fermion being described solely by D_2 and the lattice gauge field action being shifted by

$$S_{gauge} \rightarrow S_{gauge} + \Delta S. \quad (5)$$

If the shift (5) does not change the universality class, i.e., leaves the lattice theory in the right universality class for QCD, then surely the same is true for the smaller shift

$$S_{gauge} \rightarrow S_{gauge} + \frac{1}{2}\Delta S. \quad (6)$$

But this shift is equivalent to leaving S_{gauge} unchanged and changing the fermion determinant in the mixed fermion generating functional (2) by

$$\det D_1 \rightarrow (\det D_1 \det D_2)^{1/2} \quad (7)$$

We conclude that if the lattice QCD theory with mixed fermion action is in the right universality class for QCD then so is the theory where a dynamical quark is described by the 2nd taste (flavor) of the 2-taste lattice Dirac operator

$$D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix} \quad (8)$$

and with rooted fermion determinant $(\det D)^{1/2}$.

Normally there would be no reason to consider such a formulation in practice rather than just using D_1 or D_2 or the mixed fermion formulation. But it is useful to consider this formulation for theoretical investigation of lattice QCD with rooted fermion determinants – it is simpler than the relevant case of staggered fermions since the taste (flavor) interpretation is manifest from the beginning and there is no mixing between the different tastes. In the next section we will exhibit a 2-taste lattice Dirac operator of the form (8) with properties analogous to the staggered Dirac operator and for which Creutz’s objections also apply. The preceding considerations have already shown (at least heuristically) that the viability of using the rooted determinant of such an operator is assured if the related unrooted mixed fermion theory is in the right universality class for QCD.

III. A 2-TASTE LATTICE DIRAC OPERATOR WITH EXACT CHIRAL SYMMETRIES

The specific 2-taste lattice Dirac operator we will study is given in the massless case by

$$D = \begin{pmatrix} D_+ & 0 \\ 0 & D_- \end{pmatrix} \quad , \quad D_{\pm} = \gamma_{\mu} \nabla_{\mu} \pm i\gamma_5 (a\frac{1}{2}\Delta + m_5) \quad (9)$$

where a =lattice spacing, ∇_{μ} is the usual symmetrized lattice covariant derivative and Δ the usual lattice Laplace operator. For reasons discussed below we have included a mass parameter m_5 in the operator. It should not be confused with the usual mass; we introduce the latter in the usual way: the massive 2-taste Dirac operator is $D + m$. Note that D_{\pm} , and hence D , are anti-hermitian, and that in the free field case (link variables set to unity)

$$\left[D_{\pm}^{\dagger} D_{\pm} \right]_{free} = \left[\not{\nabla}^{\dagger} \not{\nabla} + (a\frac{1}{2}\Delta + m_5)^2 \right]_{free} \quad (10)$$

which shows that D_{\pm} is free of fermion doubling so D describes two lattice fermion tastes as claimed. Writing D as

$$D = (\gamma_{\mu} \otimes \mathbf{1}) \nabla_{\mu} + i(\gamma_5 \otimes \sigma_3)(a\frac{1}{2}\Delta + m_5) \quad (11)$$

we see that it has the taste-nonsinglet chiral symmetries

$$\{D, \Gamma_j\} = 0 \quad , \quad \Gamma_j = \gamma_5 \otimes \sigma_j \quad , \quad j = 1, 2 \quad (12)$$

where $\sigma_1, \sigma_2, \sigma_3$ are the Pauli matrices acting on taste space. On the other hand, D breaks the symmetry of the chiral transformation generated by $\gamma_5 \otimes \sigma_3$ (and also $\gamma_5 \otimes \mathbf{1}$ as it should to produce the axial anomaly). Consequently the pion spectrum will not be SU(2)-symmetric, so the fermion theory described by D is not equivalent at non-zero lattice spacing to a two-flavor theory with both flavors described by the same single-taste lattice Dirac operator.³

Thus D shares key properties with the massless staggered lattice Dirac operator: it is anti-hermitian and has taste-nonsinglet chiral symmetries which protect against additive mass renormalization and are expected to be spontaneously broken just like the taste-nonsinglet U(1) chiral symmetry of staggered fermions, while other chiral symmetries are explicitly

³ This is the same reasoning that was used in Ref.[4] to draw the analogous conclusion for the staggered fermion theory.

broken at non-vanishing lattice spacing. In fact the expression (11) has clear similarities with the massless staggered Dirac operator in the flavor (taste) representation [24, 25].

However, there is also a significant difference: Our operator breaks the parity and time reversal symmetries, since the “Wilson-like” term in D_{\pm} gives a pseudo-scalar term in the fermion action. Consequently, radiative corrections will generate a pseudoscalar mass term. Therefore we have included a bare pseudo-scalar mass term with mass m_5 in (9); it should be tuned to a critical negative value as the continuum limit is approached so as to cancel the pseudo-scalar mass term generated by radiative corrections and thereby restore the P and T symmetries in the continuum limit. (This is analogous to the tuning of the bare scalar mass to a critical negative value to reach the chiral limit with usual Wilson fermions.) Through this we also expect the chiral transformation generated by $\gamma_5 \otimes \sigma_3$ to become a symmetry of the 2-taste theory in the continuum limit. Usually we will suppress the m_5 -dependence of D in the notation, although sometimes we will indicate it explicitly as $D(m_5)$.

The 2-flavor theory described by $D(m_5) + m$ can be obtained from the 2-flavor Wilson fermion theory with twisted mass [26] by a flavored chiral rotation of the fields. We show this in Appendix A. However, as shown there, the symmetries of the theories have different interpretations: the chiral symmetries (12) correspond to vector symmetries in the Wilson case.

A major advantage that our setting has over the staggered one for investigating the viability of rooting is that there is a single-flavor fermion theory that our rooted theory can be explicitly compared with, namely the theory described by $D_+ + m$ (or $D_- + m$). Comparison of the rooted theory based on $D + m$ with the single-flavor theory described by $D_+ + m$ will be our main focus in this paper. Through this we will be able to counter Creutz’s objections to the rooting trick quite explicitly.

The starting point for much of Creutz’s argumentation against the rooted staggered fermion determinant is the observation that, as a consequence of its exact $U(1)$ chiral symmetry, the staggered fermion theory with mass m is equivalent to the one with mass term changed by

$$m\bar{\psi}\psi \rightarrow m\bar{\psi}\psi \cos(2\theta) + im\bar{\psi}\Gamma_5\psi \sin(2\theta) \quad (13)$$

for any θ , where Γ_5 is the operator on staggered fermion fields corresponding to γ_5 in the naive lattice fermion theory from which the staggered theory originates. See Eq.(4) of

Ref.[19]. In particular, m , $-m$ and $\pm i\Gamma_5 m$ are all physically equivalent. Therefore, the rooted staggered fermion determinant is invariant under these changes in the mass term, unlike the determinant of a genuine one-flavor lattice Dirac operator. Exactly the same is true in the present 2-taste theory when Γ_5 in (13) is replaced by our Γ_1 or Γ_2 in light of (12). Therefore, all Creutz's objections against rooting based on (13) apply just as much in our case. In the following sections we derive explicit relations between the rooted determinant formulation and single-taste theories in the present case which show that, despite Creutz's concerns, the rooted formulation does appear to be viable, or at least a good approximation when the quark masses are not too small.

IV. PROPERTIES OF THE SINGLE-TASTE THEORY AND IMPLICATIONS FOR THE ROOTED FORMULATION

In this section we derive general properties of the single-taste theories described by $D_\pm + m$ and use them to obtain significant indications of the viability of the rooted determinant $\det(D + m)^{1/2}$. Throughout the following we assume that the lattice is finite; then the vectorspace of lattice spinor fields is finite-dimensional and the fermion determinants are all finite.

A. Fermion determinants and would-be zero-modes

D_\pm in (9) satisfies

$$D_\pm \gamma_5 = -\gamma_5 D_\mp \quad (14)$$

implying an equivalence between the eigenvalue equations for D_+ and D_- :

$$D_+ \psi_\lambda = i\lambda \psi_\lambda \Leftrightarrow D_- (\gamma_5 \psi_\lambda) = -i\lambda (\gamma_5 \psi_\lambda) \quad (15)$$

Using this, we find that the rooted determinant of $D + m$ is given in terms of the eigenvalues $\{i\lambda\}$ of D_+ by

$$\det(D + m)^{1/2} = \prod_\lambda \sqrt{\lambda^2 + m^2} \quad (16)$$

Comparing this with the determinant of the single-taste Dirac operator D_+

$$\det(D_+ + m) = \prod_\lambda (i\lambda + m) \quad (17)$$

we see that

$$\det(D + m)^{1/2} = |\det(D_+ + m)| \quad (18)$$

This shows that using the rooted determinant is the same as removing the complex phase of the single-taste determinant $\det(D_+ + m)$. We will show further below that the single-taste determinant is indeed complex-valued, calculate its complex phase when m is in a “chiral region”, and discuss how the complex phase can be removed to arrive at the rooted determinant via (18). The would-be zero-modes of the 1-taste and 2-taste theories play an important role in this, and we begin by considering them in the following.

An exact zero-mode would give rise to a factor $|m|$ in (18) rather than the factor m which would appear in a genuine one-flavor fermion determinant. This difference is expected (see, e.g., [10, 11]) and is inconsequential as long as considerations are restricted to positive m . In practice though we do not expect exact zero-modes for this operator; the most one can hope for is approximate, would-be zero-modes that become exact in the continuum limit. To produce expected non-perturbative effects it is crucial that there are robust would-be zero-modes in topologically non-trivial gauge field backgrounds in accordance with the Index Theorem. These are indeed present in this case, as we will now show.

It is useful to introduce the new gamma-matrices

$$\tilde{\gamma}_\mu = -i\gamma_5\gamma_\mu \quad (19)$$

These form another representation of the Dirac algebra: $\{\tilde{\gamma}_\mu, \tilde{\gamma}_\nu\} = 2\delta_{\mu\nu}$, continue to be hermitian ($\tilde{\gamma}_\mu^\dagger = \tilde{\gamma}_\mu$) and have the same chirality matrix as before: $\tilde{\gamma}_5 = \gamma_5$. Then D_+ in (9) can be expressed as

$$\begin{aligned} D_+ &= i\gamma_5(\tilde{\gamma}_\mu\nabla_\mu + \frac{a}{2}\Delta + m_5) \\ &= i\tilde{\gamma}_5(D_{\tilde{W}} + m_5) \end{aligned} \quad (20)$$

where $D_{\tilde{W}}$ is the massless Wilson-Dirac operator constructed with the new gamma-matrices. Introducing the hermitian operator

$$H(m) = \tilde{\gamma}_5(D_{\tilde{W}} - m) \quad (21)$$

we have

$$D_+ = iH(-m_5) \quad (22)$$

so the solutions to the eigenvalue equation

$$H(m)\psi_\lambda(m) = \lambda(m)\psi_\lambda(m) \quad (23)$$

give back the eigenvalues and eigenvectors of D_+ in (15) as a special case: $\lambda = \lambda(-m_5)$, $\psi_\lambda = \psi_\lambda(-m_5)$.

From (21) we see that

$$\lambda(m_0) = 0 \Leftrightarrow D_{\tilde{W}}\psi_\lambda(m_0) = m_0\psi_\lambda(m_0) \quad (24)$$

i.e., vanishing of an eigenvalue $\lambda(m)$ at m_0 corresponds to a real eigenvalue m_0 of the Wilson-Dirac operator with eigenvector $\psi_\lambda(m_0)$. It is well-known that the would-be zero-modes of the Wilson-Dirac operator are precisely the low-lying real (necessarily positive) eigenvalue modes. As (24) shows, these correspond to crossings of the origin close to zero (i.e., at some small positive value m_0) by eigenvalues $\lambda(m)$ of $H(m)$. Furthermore, the low-lying real modes of $D_{\tilde{W}}$ have approximate \pm chirality under $\tilde{\gamma}_5$, and from (21) it is clear that the sign of the chirality is minus the sign of the slope of $\lambda(m)$ where it crosses the origin at m_0 . This is all well-known and was discussed a long time ago by Itoh, Iwasaki and Yoshié [27]. It allows a robust, integer-valued index to be defined for the Wilson-Dirac operator in terms of the spectral flow of $H(m)$ in the small m region: it is the difference between the number of negative and positive slope eigenvalue crossings. In fact this coincides with the index of the overlap Dirac operator [28]. It has been studied numerically in [27, 29], and analytically in [30, 31] where it was shown to coincide with the topological charge of the (smooth) lattice gauge field in the continuum limit in accordance with the Index Theorem.⁴

By (22)–(24) a real mode of $D_{\tilde{W}}$ with eigenvalue m_0 is an exact zero-mode of $D_+(m_5)$ when we set $m_5 = -m_0$. For an ensemble of lattice gauge fields generated at sufficiently small bare coupling (or with a sufficiently improved lattice gauge action) the low-lying real eigenvalues of $D_{\tilde{W}}$ cluster around a critical (positive) value m_c – see, e.g., [27]. We henceforth

⁴ The robustness of low-lying real eigenvalue modes and index of the Wilson-Dirac operator is ensured by the property that in sufficiently smooth backgrounds the eigenvalues cannot vary arbitrarily under deformations of the background but are constrained to be close to zero. An upper bound can be analytically derived when the plaquette variables satisfy a bound $\|1 - U_{\mu\nu} - 1\| < \epsilon$ [32, 33]. More generally, a bound constraining the real eigenvalues to lie in neighborhoods of 0, $2/a$, $4/a$, $6/a$, $8/a$ can be derived in this case [34].

tune m_5 so that

$$m_5 = -m_c. \quad (25)$$

Consequently the eigenvalues and eigenvectors of D_+ are $i\lambda(m_c)$ and $\psi_\lambda(m_c)$, respectively. Then the would-be chiral zero-modes of $D_{\tilde{W}}$ are in one-to-one correspondence with would-be chiral zero-modes of D_+ . This is seen as follows. A low-lying real mode of $D_{\tilde{W}}$ with eigenvalue m_0 is a zero-mode $\psi_\lambda(m_0)$ for $H(m_0)$ with approximately definite chirality. Since $\lambda(m_0) = 0$ and m_0 is very close to m_c it follows that $\lambda(m_c)$ is very small, and the corresponding eigenvector $\psi(m_c)$ is very close to $\psi(m_0)$ and therefore has the same approximate chirality. Recall that the sign of the chirality is the opposite of the sign of the slope of $\lambda(m)$ at $m = m_0$. Therefore, \pm chirality corresponds to the sign of $\lambda(m_c)$ being \pm if $m_c < m_0$ and \mp if $m_c > m_0$.

Thus, with m_5 tuned as dictated by (25), the low-lying modes of D_+ are generically would-be chiral zero-modes; they are robust since they are tied to the would-be chiral zero-modes (i.e., the low-lying real modes) of the Wilson-Dirac operator $D_{\tilde{W}}$. By (15) the same is true for D_- . Note that a would-be chiral zero-mode for the Wilson-Dirac operator corresponds to would-be chiral zero-modes for each of D_+ and D_- with the *same* chirality; consequently it corresponds to two would-be chiral zero-modes for D with the same chirality. Thus we have established that D_+ , D_- , and D all have robust would-be chiral zero-modes in sufficiently smooth gauge backgrounds, and that the index defined from these equals the topological charge Q of the gauge background (or $2Q$ in the case of the 2-taste operator D) in accordance with the Index Theorem, since this holds for the Wilson-Dirac operator.

The tuning of m_5 dictated by (25) is also the appropriate one for restoring in the continuum limit the P and T symmetries and the chiral symmetry of the 2-taste theory generated by $\gamma_5 \otimes \sigma_3$. Restoring these symmetries means tuning m_5 so that the effective pseudo-scalar mass term vanishes. The usual signal for the vanishing of an effective mass term (scalar or pseudo-scalar) is divergence of the propagator, and from the discussion leading to (25) it is clear that this tuning produces the desired divergence in the present case. (It is analogous to the tuning of the bare mass to a critical negative value to reach the chiral limit with Wilson fermions.)

Returning now to the fermion determinants, we first note that in approaching the chiral

limit the scalar mass m should be tuned such that

$$|\lambda_{low}| \ll |m| \ll |\lambda_{nonlow}| \quad (26)$$

where λ_{low} refers to the eigenvalues of the would-be zero-modes and λ_{nonlow} refers to all the other eigenvalues. The reason is to achieve appropriate near-chiral limit mass dependence in the fermion determinants: from (16)–(17) we see that (26) is necessary and sufficient to get

$$\det(D_+ + m) \approx \prod_{\lambda_{low}} m \prod_{\lambda_{nonlow}} i\lambda_{nonlow} \quad (27)$$

$$\det(D + m)^{1/2} \approx \prod_{\lambda_{low}} |m| \prod_{\lambda_{nonlow}} |\lambda_{nonlow}| \quad (28)$$

To compare the rooted determinant with the single-taste determinant $\det(D_+ + m)$ we need to determine the complex phase of the latter. We now calculate it for m in the chiral region (26), starting from

$$\frac{\det(D_+ + m)}{|\det(D_+ + m)|} \approx \prod_{\lambda_{low}} \frac{m}{|m|} \prod_{\lambda_{nonlow}} i \frac{\lambda_{nonlow}}{|\lambda_{nonlow}|} \quad (29)$$

where negligible terms $\sim \frac{\lambda_{low}}{m}$ and $\sim \frac{m}{\lambda_{nonlow}}$ have been dropped. To evaluate this we will use

$$\prod_{\lambda_{nonlow}} i = \prod_{\lambda_{low}} (-i) \quad (30)$$

which follows from $\prod_{\lambda} i = 1$, a consequence of the fact that the dimension of the vectorspace of lattice spinor fields is a multiple of 4. Now recall that the eigenvalues λ_{nonlow} are the values at $m = m_c$ of $\lambda_{nonlow}(m)$. Generically these do not cross zero in the small m region; in particular they do not cross zero as m varies from 0 to m_c . Therefore,

$$\prod_{\lambda_{nonlow}} \frac{\lambda_{nonlow}(m_c)}{|\lambda_{nonlow}(m_c)|} = \prod_{\lambda_{nonlow}} \frac{\lambda_{nonlow}(0)}{|\lambda_{nonlow}(0)|} = \prod_{\lambda_{low}} \frac{\lambda_{low}(0)}{|\lambda_{low}(0)|} \quad (31)$$

where the last equality follows from $\prod_{\lambda} \frac{\lambda(0)}{|\lambda(0)|} = 1$, a consequence of the known fact that $Tr \frac{H(0)}{|H(0)|} = 0$; see, e.g., [34]. On the other hand, the eigenvalues $\lambda_{low}(m)$ do cross zero in the small positive m region. If $\lambda_{low}(0) > 0$ then $\lambda_{low}(m)$ has negative crossing slope, corresponding to a positive chirality would-be zero-mode by our previous discussion. Similarly, $\lambda_{low}(0) < 0$ implies a would-be zero-mode with negative chirality. It follows that

$$\prod_{\lambda_{low}} \frac{\lambda_{low}(0)}{|\lambda_{low}(0)|} = (-1)^{n_-} \quad (32)$$

where n_{\pm} denotes the number of \pm chirality would-be zero-modes. This together with (31) and (30) leads to

$$\prod_{\lambda_{nonlow}} i \frac{\lambda_{nonlow}}{|\lambda_{nonlow}|} = i^{-Q} \quad (33)$$

where

$$Q = n_+ - n_- \quad (34)$$

is the index of the would-be chiral zero-modes and coincides with the topological charge in sufficiently smooth gauge backgrounds as discussed earlier. Using this in (29) we finally obtain

$$\frac{\det(D_+ + m)}{|\det(D_+ + m)|} \approx i^{-\frac{m}{|m|}Q} = e^{-i\frac{m}{|m|}\frac{\pi}{2}Q} \quad (35)$$

The equality becomes exact in the limit $\frac{\lambda_{low}}{m} \rightarrow 0$, $\frac{m}{\lambda_{nonlow}} \rightarrow 0$, which should be regarded as the chiral limit in this setting. The prospects for the possibility of being able to take this limit (in principle) are discussed in the concluding section.

Thus for m in the chiral region (26) the effect of the complex phase of $\det(D_+ + m)$ is to shift the QCD theta-vacuum angle by $\theta \rightarrow \theta - \frac{m}{|m|}\frac{\pi}{2}$. Since the physical theta-vacuum angle must be zero (or extremely close to zero) [35], the bare theta-vacuum angle in the lattice QCD theory must be chosen such that the shifted one vanishes. This is equivalent to having trivial theta vacuum and replacing the fermion determinant (with $m > 0$) by

$$\det(D_+ + m) \rightarrow e^{i\frac{\pi}{2}Q} \det(D_+ + m) \quad (36)$$

which is essentially the same as

$$\det(D_+ + m) \rightarrow |\det(D_+ + m)| = \det(D + m)^{1/2} \quad (37)$$

in the chiral region. This strongly indicates the viability of using the rooted determinant to represent the determinant for a single quark flavor in the present case.

As a further indication of the viability of the rooted determinant we see from (20) with (25) that

$$\det D_+ = \det(D_W - m_c). \quad (38)$$

Since the Wilson fermion determinant is real and positive, this shows that $\det(D + m)^{1/2}$ coincides at $m = 0$ with the Wilson fermion determinant with bare mass tuned to precisely the negative critical value which it should have in the chiral limit. Therefore, for very small m in the chiral region (26), the rooted determinant is very close to the chiral limit of the Wilson fermion determinant.

Flipping the sign of m has the effect of complex conjugation on the phase factor in (35). We note in passing that this is a general property the single-taste fermion determinant: From (17) and (15) we easily find

$$\det(D_+ - m) = \det(D_+ + m)^* = \det(D_- + m) \quad (39)$$

B. Origin of the complex phase

For the rooted formulation to be viable, the low energy physics it describes should be the same as when the fermion is described by $D_+ + m$ with a bare theta term included in the lattice QCD action to cancel the one produced by $\det(D_+ + m)$. For this to hold, the complex phase should originate from the ultra-violet part of the spectrum of $D_+ + m$, so that it is not a manifestation of low energy aspects of the fermion formulation described by $D_+ + m$. We show this to be the case in the following.

In sufficiently smooth gauge backgrounds where the Index Theorem relation between chirality of would-be zero-modes and topological charge holds, it is known that for each would-be chiral zero-mode of the Wilson-Dirac operator there are 15 “doubler” modes [27, 34]. These are eigenvectors of D_W with approximately definite chirality and with large (positive) real eigenvalues clustered around specific values: If the approximate chirality of the zero-mode is \pm then the associated real eigenmodes consist of four eigenvectors with eigenvalues $\approx 2/a$ and chirality \mp ; six eigenvectors with eigenvalues $\approx 4/a$ and chirality \pm ; four eigenvectors with eigenvalues $\approx 6/a$ and chirality \mp , and one eigenvector with eigenvalue $\approx 8/a$ and chirality \pm [34]. By (24) this implies a corresponding family $\{\psi_j(m)\}_{j=0,1,\dots,15}$ of eigenvectors, $H(m)\psi_j(m) = \lambda_j(m)\psi_j(m)$, with each $\lambda_j(m)$ vanishing at a value m_j close to $2p/a$ for some $p \in \{0, 1, 2, 3, 4\}$. There are $\frac{4!}{p!(4-p)!}$ j ’s for each p , and $\psi_j(m_j)$ has the approximate chirality $\pm(-1)^p$ under γ_5 .

Noting that $H(m_c)$ can be written for each j as $H(m_c) = H(m_j) + (m_j - m_c)\gamma_5$ we see that

each $\psi_j(m_j)$ is an approximate eigenvector for $H(m_c)$, and therefor also for $D_+ = iH(m_c)$:

$$H(m_c)\psi_j(m_j) \approx \pm(-1)^p(m_j - m_c)\psi_j(m_j). \quad (40)$$

Since $m_c \approx 0$ it follows that, generically, the spectrum $\{i\lambda\}$ of D_+ contains 15 “doubler” eigenvalues associated with each would-be zero-eigenvalue; four of them are $\approx \mp i2/a$; six of them are $\approx \pm i4/a$; four of them are $\approx \mp i6/a$; and the final one is $\approx \pm i8/a$ where \pm is the chirality of the would-be zero-mode. The contribution of these to the phase factor in (29) is

$$\prod_{j=1}^{15} i \frac{\lambda_j}{|\lambda_j|} = (\mp i)^4 (\pm i)^6 (\mp i)^4 (\pm i) = \mp i \quad (41)$$

It follows that the total contribution to the phase factor from the doubler modes of all the would-be zero-modes is $(-i)^{n_+} i^{n_-} = i^{-Q}$. This reproduces precisely the phase factor in (33), which for $m > 0$ gives the complex phase of the determinant in (35). Thus we have found that, at least when m is in the chiral region, the complex phase of $\det(D_+ + m)$ originates entirely from the would-be doubler modes associated with the would-be zero-modes of D_+ . An analogous result holds for $\det(D_- + m)$. The doubler mode eigenvalues are $\sim 1/a$, so we conclude that the complex phases of the determinants are not connected with the low energy physics of the fermion tastes described by $D_+ + m$ and $D_- + m$.

C. Determinant phase factor and axial anomaly in the classical continuum limit

A classical continuum limit version of our determinant phase factor result (35) arises as a special case of a previous result of Seiler and Stamatescu (SS) [36]. They considered the $m_5 = 0$ case of the lattice Dirac operator

$$D_\theta = \gamma_\mu \nabla_\mu + e^{i\theta\gamma_5} (a \frac{r}{2} \Delta + m_5). \quad (42)$$

which coincides with our D_\pm for $\theta = \pm\pi/2$. SS showed that the fermion determinant $\det(D_\theta + m)$ produces a theta-vacuum term $e^{-i\theta Q}$ in the classical continuum limit (with $m > 0$). A simple consequence of their specific result, Eq.(19) of [36], is⁵

$$\lim_{a \rightarrow 0} \frac{\det(D_\theta^A + m)}{|\det(D_\theta^A + m)|} = e^{-i\theta Q} \quad (43)$$

⁵ The minus sign in the exponent of $e^{-i\theta Q}$ is erroneously absent in Eq.(19) of [36]; it should be present due to minus sign in their Eq.(22).

where the gauge background is the lattice transcript of a smooth continuum gauge field A (satisfying certain technical conditions) with topological charge Q . For $\theta = \pi/2$ this is obviously a classical continuum limit version of our result (35) with $m > 0$.

The result (43) is obtained as a straightforward consequence of another result of SS, namely that $D_\theta + m$ reproduces the correct axial anomaly in the classical continuum limit for all values of θ . This implies in particular that fermions described by $D_+ + m$ and $D_- + m$ both reproduce the correct axial anomaly, so the same is true for the 2-flavor theory described by our $D + m$. We emphasize that both tastes reproduce the correct anomaly with the right sign; they do not have opposite signs and so Creutz's concern about cancellation of anomalies [19] is not realized here. Although the considerations of SS were without m_5 , their results extend almost immediately to $m_5 \neq 0$. This is because m_5 , just like m , appear in the final axial anomaly expression through the dimensionless quantities am_5 and am and hence drop out in the $a \rightarrow 0$ limit. (However, m plays the role of infrared regulator in intermediate stages of the evaluation and must therefore be non-vanishing and positive.) Here m_5 and m may either be constant or tuned as a function of the lattice spacing as long as $am_5 \rightarrow 0$, $am \rightarrow 0$ for $a \rightarrow 0$.

V. PSEUDOSCALAR MESON PROPAGATOR IN THE ROOTED FORMULATION

We now consider the pseudoscalar meson propagator, more specifically its disconnected piece $G^{DC}(x, y)$, which is supposed to solve the $U(1)$ problem by being non-vanishing in the chiral limit in topologically nontrivial gauge field backgrounds and thereby partially cancelling the connected piece, resulting in quicker decay, and hence a large mass. This cancellation, which was already verified a long time ago in the chiral limit with Wilson fermions [27], requires that $G^{DC}(x, y)$ in a fixed topologically nontrivial gauge background develops a singularity $\sim 1/m^2$ in the chiral limit, produced by the (would-be) zero-modes of the (lattice) Dirac operator.

For simplicity we restrict to the one flavor case; then, with our 2-taste D we have

$$G^{DC}(x, y) = \frac{1}{2}\text{tr}[(D + m)^{-1}(x, x)(\gamma_5 \otimes \mathbf{1})] \frac{1}{2}\text{tr}[(D + m)^{-1}(y, y)(\gamma_5 \otimes \mathbf{1})] \quad (44)$$

We have replaced $\text{tr} \rightarrow \frac{1}{2}\text{tr}$ compared to the usual expression to take account of the two

tastes of D . It suffices to consider just one of the factors $\frac{1}{2}\text{tr}[\cdots]$. A simple calculation using (14)-(15) gives

$$\frac{1}{2}\text{tr}[(D + m)^{-1}(x, x)(\gamma_5 \otimes \mathbf{1})] = \sum_{\lambda} \frac{m}{\lambda^2 + m^2} \psi_{\lambda}^{\dagger}(x) \gamma_5 \psi_{\lambda}(x) \quad (45)$$

Exactly the same expression can be (formally) derived in the continuum from $\not{D}\psi_{\lambda} = i\lambda\psi_{\lambda}$ using the fact that $\not{D}(\gamma_5\psi_{\lambda}) = -i\lambda(\gamma_5\psi_{\lambda})$. However, in the present lattice setting we do not have exact zero-modes in general so (45) and hence $G^{DC}(x, y)$ vanish at $m = 0$. (This can also be seen directly from the chiral symmetries in (12) since Γ_j ($j = 1, 2$) commutes with $\gamma_5 \otimes \mathbf{1}$. The situation is the same for staggered fermions – see Sect. VIII.F of Ref.[27].) Clearly the $m \rightarrow 0$ limit should not be taken before the continuum limit here.⁶ The situation is different from Wilson fermions where the chiral limit can be reached by tuning the mass to a critical negative value [27]. In the present case, reaching the chiral limit requires being able to choose m in the same way as in our discussion of the fermion determinants in the previous section, namely, it should be in the “chiral region” (26). Then (45) becomes

$$\frac{1}{2}\text{tr}[(D + m)^{-1}(x, x)(\gamma_5 \otimes \mathbf{1})] \approx \sum_{\lambda_{low}} \frac{1}{m} \psi_{\lambda_{low}}^{\dagger}(x) \gamma_5 \psi_{\lambda_{low}}(x) \quad (46)$$

which gives the correct chiral limit behavior of (45) and hence also $G^{DC}(x, y)$. The fact that only the would-be zero-modes contribute in (46) fits well with the observation from previous numerical studies that G^{DC} is essentially given by the contribution from low-lying modes – this was seen for staggered fermions in [40] and for Wilson fermions using the Hermitian Wilson-Dirac operator in [41].

From (46) and (28) we see that in the chiral region (26) with positive m the weighted propagator in the rooted theory, $\det(D + m)^{1/2} G^{DC}(x, y)$, has the same form and mass dependence as obtained from the 't Hooft vertex in the continuum setting. (This is clear, e.g., from the description of the latter given in [21].) This is clearly not the case for values of m which are smaller than specified in (26) though.

VI. CONCLUDING DISCUSSION

In the rooted fermion formulation based on $D + m$ one would expect that any problem connected with chirality would show up most clearly in the “chiral limit” of small bare mass

⁶ The necessity of taking continuum limit before chiral limit is well-known for staggered fermions [37, 38, 39].

m . We have found no sign of this, having derived quite explicit indications of the viability of the rooted formulation when the bare mass is positive and in the “chiral region” (26):

$$|\lambda_{low}| \ll m \ll |\lambda_{nonlow}| \quad (47)$$

and in particular in the “chiral limit”

$$\frac{\lambda_{low}}{m} \rightarrow 0 \quad , \quad \frac{m}{\lambda_{nonlow}} \rightarrow 0 \quad (48)$$

The existence of the chiral region and limit requires a gap in the eigenvalue spectrum of D between the eigenvalues $\{i\lambda_{low}\}$ of the would-be zero-modes and the other eigenvalues $\{i\lambda_{nonlow}\}$. It is plausible that such a gap will open up as the continuum limit (bare coupling $g \rightarrow 0$) is approached: In this limit the fluctuations of the low-lying real eigenvalues of the Wilson-Dirac operator around a critical value m_c should become smaller and smaller; then the same is true for the fluctuations of $\{\lambda_{low}\}$ around zero when m_5 is tuned to $-m_c(g)$ (cf. §4). Setting

$$f_1(g) := \max\{|\lambda_{low}|\} \quad , \quad f_2(g) := \min\{|\lambda_{nonlow}|\} \quad (49)$$

we expect

$$\frac{f_1(g)}{f_2(g)} \rightarrow 0 \quad \text{for } g \rightarrow 0 \quad (50)$$

Then, tuning m as a function of the bare coupling by, e.g.,

$$m(g) = (f_1(g)f_2(g))^{1/2} \quad (51)$$

the chiral limit (48) is reached as the continuum limit $g \rightarrow 0$ is taken. This implies that a chiral region (47) exists for sufficiently small g (and also at larger g for highly improved versions of the lattice actions).

While the requirement $m > 0$ for the bare mass has been widely recognized (e.g., in the reviews [10, 11])⁷, we have found here that a more stringent condition is required:⁸

$$m \gg \max\{|\lambda_{low}|\} \quad (52)$$

⁷ There is however a possibility of extending the rooted formulation with positive m to general complex-valued m via the introduction of a theta term, as discussed in the staggered fermion case in Ref. [42].

⁸ This condition is not at all surprising, and in fact the necessity of it could already be inferred in the staggered fermion case from the remarks in sect. VIII.F of [27].

In a lattice formulation of QCD with the fermion determinant for each dynamical quark represented by a rooted determinant the dependence of each bare mass m_q on g is fixed by renormalization conditions; e.g., by requiring that the lattice QCD theory gives specified values for a selection of hadronic mass ratios. In connection with this, Creutz has argued [43] that the notion of chiral limit for a single light quark (in practice the up quark) is physically meaningless when the other quarks remain massive: He argues that non-perturbative instanton effects will produce renormalization scheme-dependent additive corrections to the light quark mass. If this is the case then $m_q = 0$ is a scheme-dependent statement for the bare mass of the light quark. Then there is no physical reason why the bare mass must remain positive in a given scheme (i.e., for a given choice of renormalization conditions) as the continuum limit is approached, hence the requirement (52) may be violated, in which case the rooted formulation may fail. On the other hand, if the u and d quarks are taken to have degenerate bare mass then the pion spectrum is degenerate and the chiral limit is physically well-defined as the limit where the pions become massless. In this case we can expect to be able to approach this limit from within the chiral region (47). This applies not only for the present formulation (where the product of the degenerate u and d determinants are safely represented by the 2-flavor fermion determinant $\det(D + m)$) but also for the staggered formulation where the determinant product is represented by the square root of the staggered fermion determinant.

Expressions analogous to (17) for the rooted determinant and (45) for $G^{DC}(x, y)$ hold for staggered fermions since the eigenvalues of the massless staggered Dirac operator come in pairs $\pm i\lambda$. The present case is more explicit, since the eigenvalues $\{i\lambda\}$ are those of a bona fide single-taste lattice Dirac operator D_+ , whereas no such origin is known for the eigenvalues of the staggered Dirac operator. Nevertheless, the chiral limit issues discussed here are the same for staggered fermions. So achieving (47)–(48) in the staggered fermion case is also required for taking the chiral limit there. It is encouraging with regard to this that numerical studies with improved staggered fermions find a clear gap in the spectrum between the low-lying would-be zero-eigenvalues and the remainder of the spectrum [44, 45, 46].

Having seen in §4 that the 2-taste lattice Dirac operator D has robust would-be chiral zero-modes in topologically non-trivial gauge backgrounds in accordance with the Index Theorem, a natural question is whether the same is true in the case of staggered fermions. The numerical studies in [44, 45] strongly indicate that this is the case. In fact, a version

of the techniques used in this paper, supplemented with further calculations, enables the robust would-be zero-mode result here to also be established for staggered fermions, thereby providing a theoretical basis for the numerical results of [44, 45]. This will be presented in a forthcoming paper.

The 2-flavor fermion formulation specified by the lattice operator D introduced here is mathematically equivalent to twisted mass Wilson fermions, but the interpretation of the symmetries is different: Two of the flavored vector symmetries in the Wilson case correspond to the chiral symmetries (12) in our case. Other 2-flavor fermion formulations with flavored chiral symmetry have recently appeared [47, 48], inspired by graphene structure. Their properties were studied in [49] where a general argument was made that 2-flavor (“minimally doubled”) fermion formulations with an exact chiral symmetry must necessarily violate parity or time reversal symmetry. The formulation based on D in this paper is another example of this: it has two exact (flavored) chiral symmetries and violates P and T symmetry due to a pseudoscalar term in the action.

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APPENDIX A: RELATION TO TWISTED MASS WILSON FERMIONS

The twisted mass Wilson formulation for two lattice fermion flavors has the action [26]

$$S_{tm} = \bar{\chi}(\gamma_\mu \nabla_\mu + a_2^r \Delta + m + i\mu\gamma_5\sigma_3)\chi. \quad (\text{A1})$$

Noting that

$$i\mu\gamma_5\sigma_3 = -\mu e^{-i\alpha\gamma_5\sigma_3}, \quad \alpha = \pi/2 \quad (\text{A2})$$

we see that the flavored chiral rotation of the fields

$$\chi = e^{i\alpha\gamma_5\sigma_3/2} \psi \quad , \quad \bar{\chi} = \bar{\psi} e^{i\alpha\gamma_5\sigma_3/2} \quad (\text{A3})$$

leads to

$$S_{tm} = \bar{\psi}(\gamma_\mu \nabla_\mu + i\gamma_5\sigma_3(a\frac{r}{2}\Delta + m) - \mu)\psi . \quad (\text{A4})$$

This coincides with the action for our 2-flavor theory,

$$S = \bar{\psi}(D(m_5) + m)\psi \quad (\text{A5})$$

with

$$m_5 \rightarrow m \quad , \quad m \rightarrow -\mu \quad (\text{A6})$$

At $m = 0$ our formulation has the exact flavored chiral symmetries generated by $\Gamma_j = \gamma_5\sigma_j$ $j=1, 2$ (recall (12)). By (A4)–(A6) $m = 0$ in our theory corresponds to $\mu = 0$ in the twisted mass theory. But from (A1) we see that this is just the usual 2-flavor Wilson theory with mass m . Thus the symmetries, which in our theory are flavored chiral symmetries, correspond in the twisted mass setting to non-chiral symmetries of the usual 2-flavor massive Wilson theory with vanishing twisted mass. Specifically, these symmetries, which leave $\bar{\chi}(D_W + m)\chi$ invariant, are the vector symmetries

$$\delta\chi = -i\sigma_j\sigma_3\chi \quad , \quad \delta\bar{\chi} = \bar{\chi}i\sigma_j\sigma_3 \quad (\text{A7})$$

for $j = 1, 2$.

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